MAPS OF ZEROES OF THE GRAND CANONICAL PARTITION FUNCTION IN A STATISTICAL MODEL OF HIGH ENERGY COLLISIONS

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Abstract

Theorems on zeroes of the truncated generating function in the complex plane are reviewed. When examined in the framework of a statistical model of high energy collisions based on the negative binomial (Pascal) multiplicity distribution, these results lead to maps of zeroes of the grand canonical partition function which allow to interpret in a novel way different classes of events in pp collisions at LHC c.m. energies.

1 Introduction

Following previous work [1], the multiplicity distribution (MD) generating function in the dummy variable z,

$$G(z) = \sum_{n=0}^{\infty} P_n z^n \tag{1}$$

has been recognised to be related to the grand canonical partition function of a system of n particles in statistical mechanics when z is identified with the fugacity variable; P_n is here the probability of detecting n charged particles

in full phase space $(\sum_{n=0}^{\infty} P_n = 1)$ and it is linked to the canonical partition function.

It has to be stressed that in a realistic experiment n will never become infinity. Let us call M the maximum finite value of n which can be detected in an experiment. The generating function G(z) in this case is reduced to a polynomial of degree M in z:

$$G_M(z) = \sum_{n=0}^{M} P_n z^n. \tag{2}$$

Let us now consider the algebraic equation

$$G_M(z) = 0 (3)$$

in the complex z-plane. In the first place, notice that none of the roots z_i (i = 1, ..., M) of equation (3) can be real and positive, since the P_n in (2) are positive for any n. In the second place, recall that the M-truncated generating function (as any polynomial) can be factorised in terms of its roots as follows:

$$G_M(z) = P_M \prod_{i=1}^{M} (z - z_i).$$
 (4)

By applying these considerations to phase transitions of a lattice gas (and of the Ising model), C.N. Yang and T.D. Lee [2] have found that the roots z_i lie on a circle centered at the origin of the complex z-plane. The circle is open in a small sector bisected by the positive real axis; no zero lies in that sector. When M is odd, at least one root is real: it will of course be on the negative side. $G_M(z)$ turns out to be an analytic function along the positive real axis for any M. A phase transition in the sense of a non analytic behaviour of the thermodynamical functions (like pressure for instance) can only occur at points of the positive real z axis which are "in the thermodynamical limit" accumulation points of the zeroes of the algebraic equation (3). For $M \to \infty$, one should expect in general that the zeroes become closer and closer to the real positive axis and that the distance between the zeroes vanishes.

The first application of these ideas to particle production goes back to the 70's [3], but the field flourished again (results were obtained in the context a discrete approximation to QCD cascades [4]) in 1995, when E. De Wolf [5] studied, using the JETSET Monte Carlo generator, the zeroes of the generating function of the n-charged particle multiplicity distribution in e^+e^- annihilation in the y-rapidity interval |y| < 0.5 at 1000 GeV c.m. energy. The zeroes were found to lie on a circle of approximately unit radius centered at the origin of the complex z-plane. Intriguing questions were also raised on

the development of this approach in different models and in different classes of events.

After recalling and extending the main theorems on the subject, the present paper explores the properties of the distribution of zeroes in high energy collisions in the framework of the weighted superposition mechanism of different classes of events: each class is described by a Negative Binomial (Pascal) MD, whose characteristic parameters are \bar{n} , the average charged particle multiplicity, and k, linked to the dispersion D by $k = \bar{n}^2/(D^2 - \bar{n})$.

2 Maps of zeroes in the complex plane and the class of power series distributions.

In 1997, T.C. Brooks, K.L. Kowalsky and C.C. Taylor [6] applied the Eneström-Kakeya theorem [7] to the scaled *M*-truncated generating function

$$G_M(\lambda z) = \sum_{n=0}^{M} c_n z^n \tag{5}$$

with coefficients given by $c_n = \lambda^n P_n$ and the parameter λ defined as the minimum of the ratio of two consecutive c_n coefficients:

$$\lambda = r[n_{\min}] = \min[P_n/P_{n+1}] = P_{n_{\min}}/P_{n_{\min}+1}.$$
 (6)

The coefficients c_n , for n = 0, 1, ..., M, are real and positive and satisfy the condition

$$c_0 \ge c_1 \ge \cdots \ge c_M$$

required by the Eneström-Kakeya (EK) theorem in order to ensure that $G_M(\lambda z)$ differs from zero in the complex z-plane for |z| < 1. Equation (5) can be rewritten in terms of the variable w = 1/z as

$$G_M(\lambda z) = z^M g_M(w), \tag{7}$$

with

$$g_M(w) = \sum_{m=0}^M w^m c_m \tag{8}$$

and

$$c_m = \lambda^{M-m} P_{M-m}. (9)$$

By choosing now the maximum of the ratio between two consecutive c_m coefficients:

$$\lambda = r[n_{\text{max}}] = \max[P_n/P_{n+1}] = P_{n_{\text{max}}}/P_{n_{\text{max}}+1}$$

one finds that the coefficients c_m satisfy once again the EK theorem: they are indeed real and positive and ordered following the rule $c_0 \geq \cdots \geq c_m \geq \cdots \geq c_M$. Therefore $g_M(w)$ differs from zero for |w| < 1 and the zeroes of $g_M(w)$ lie necessarily in the region $|w| \geq 1$.

Accordingly, all the zeroes of the truncated generating function $G_M(z)$ fall in the annular region in the complex z-plane centered at the origin and limited by $r[n_{\min}]$ and $r[n_{\max}]$. The positive real axis is of course excluded.

The mentioned theorem turns out to be quite useful when applied to the class of power series distributions, defined as follows:

$$P_n = c_n b^n P_0. (10)$$

The corresponding M-truncated generating function is

$$G_M(z) = A_M P_0 \sum_{n=0}^{M} c_n b^n z^n = A_M P_0 \sum_{n=0}^{M} c_n (bz)^n$$
(11)

where $A_M = \left(\sum_{n=0}^M P_n\right)^{-1}$ is a normalisation factor. In the polynomial (11), the term P_0 can be neglected and bz replaced by the variable u, producing a new scaled generating function in u:

$$H_M(u) = \sum_{n=0}^{M} c_n u^n \tag{12}$$

which —as we will see in the following— is of particular interest for classifying different classes of events described in terms of NB (Pascal) MD with different parameters. In fact, applying the above considerations to the generating function

$$G^{[NB]}(z) = \sum_{n=0}^{\infty} P_n^{[NB]} z^n = \left(\frac{k}{k + \bar{n}(1-z)}\right)^k$$
 (13)

with

$$P_n^{[NB]} = \frac{k(k+1)\dots(k+n-1)\bar{n}^n k^k}{n!(\bar{n}+k)^{n+k}},$$
(14)

leads to the M-truncated version of $G^{[NB]}(z)$:

$$G_M^{[NB]}(z) = A_M^{[NB]} \sum_{n=0}^M P_n^{[NB]} z^n = A_M^{[NB]} \sum_{n=0}^M \prod_{i=1}^n \left(\frac{k+i-1}{i}\right) P_0 b^n z^n$$
 (15)

with $b = \frac{\bar{n}}{\bar{n}+k}$. Notice that in (13), $G^{[NB]}(z)$ has a singularity for z = 1/b.

By defining now in (15)

$$c_n^{[NB]} = \prod_{i=1}^n \left(\frac{k+i-1}{i} \right)$$
 (16)

and

$$bz = u$$
,

the new renormalised generating function, neglecting the inessential factor P_0 , becomes

$$H_M^{[NB]}(u) = A_M^{[NB]} \sum_{n=0}^M \prod_{i=1}^n \left(1 + \frac{k-1}{i} \right) u^n = A_M^{[NB]} \sum_{n=0}^M c_n^{[NB]} u^n.$$
 (17)

Notice that the not-truncated version $H^{[NB]}(u)$ of (17) has a singularity at u=1. Relation (17) has been used in its not-truncated form in Ref. [1] where $c_n^{[NB]}$ has been identified with the *n*-particle canonical partition function; $H_M^{[NB]}(u)$ is in this framework the truncated grand canonical partition function. It follows that if parameter k is less than one (as in the case of the third class of events in pp collisions at 14 TeV c.m. energy [9]), then the coefficients $c_n^{[NB]}$ are all real and positive, and decrease starting from $c_0^{[NB]}$. The conditions for the applicability of the EK theorem are therefore also here satisfied, and the zeroes of the scaled generating function (17) lie all outside the circle of unit radius |u| = 1.

This situation should be contrasted with the application of the EK theorem when the parameter k is greater than one (as in the case of the soft and semi-hard classes of events in pp collisions [8]). In this case in fact, the coefficients $c_n^{[NB]}$ are in increasing order and the zeroes lie all inside the circle of unit radius.

As indicated in [7] and shown in [6], for the (not-rescaled) NB (Pascal) MD Eq. (15), one finds

$$r[n] = \frac{P_n^{[NB]}}{P_{n+1}^{[NB]}} = \frac{1}{b} \left(\frac{n+1}{n+k} \right); \tag{18}$$

thus all zeroes of the algebraic equation of the M-truncated generating function (3) lie inside the annular region of the complex z-plane delimited by $r[n_{\min}]$ and $r[n_{\max}]$, with

$$r[n_{\text{max}}] = \frac{1}{b} \left(\frac{M+1}{M+k} \right) \le |z| \le r[n_{\text{min}}] = \frac{1}{kb} \equiv \frac{1}{a} \quad (k < 1)$$
 (19)

and

$$r[n_{\min}] = \frac{1}{kb} = \frac{1}{a} \le |z| \le r[n_{\max}] = \frac{1}{b} \left(\frac{M+1}{M+k}\right) \quad (k > 1).$$
 (20)

Notice that $r[n] \to \frac{1}{b}$ when $n \to \infty$, and $r[n] \to 1$ when $\bar{n} \gg k$ (i.e. $b \to 1$). In the rescaled version (17), $r[n] = \frac{n+1}{n+k}$: it tends to 1 when $n \to \infty$ with constant k. It is remarkable that for k = 1, r[n] is also equal to one and all zeroes lie on the circle of unit radius, the u = 1 point being excluded (see Figures 1 and 2).

The role of parameter a in the case of the NB (Pascal) MD is underlined by the fact that the sum of the inverse of the zeroes of the algebraic equation (3) is given by

$$\sum_{i=1}^{M} \frac{1}{z_i} = -\frac{P_1}{P_0}. (21)$$

Recall in fact that

$$\prod_{i=1}^{M} z_i = (-1)^M \frac{P_0}{P_M}$$

and also that the sum of (n-1) by (n-1) product of zeroes equals to

$$(-1)^{n-1} \frac{P_{M-(n-1)}}{P_M};$$

for example for M=3 one gets

$$z_1 z_2 + z_1 z_3 + z_2 z_3 = (-1)^2 \frac{P_1}{P_3}.$$

It follows that

$$\sum_{i=1}^{M} \frac{1}{z_i} = \frac{(-1)^{M-1} P_{M-(M-1)} / P_M}{(-1)^M P_0 / P_M} = -\frac{P_1}{P_0}.$$

Notice that for the NB (Pascal) MD, Eq. (21) becomes

$$\sum_{i=1}^{M} \frac{1}{z_i} = -b \, k = -\frac{\bar{n}k}{\bar{n}+k} = -a. \tag{22}$$

Equation (21) is indeed a general property of polynomials and is independent of the value of M. In the u-rescaled version, one has

$$\sum_{i=1}^{M} \frac{1}{u_i} = -k. (23)$$

In addition, it should be pointed out that the NB parameters of the coefficients of the M-truncated generating function (15), namely \bar{n}_M and k_M , can be calculated directly from the zeroes of equation (3). One finds:

$$\bar{n}_M = \sum_{i=1}^M \frac{1}{1 - z_i} \tag{24}$$

and

$$k_M = -\frac{\left(\sum_{i=1}^M \frac{1}{1-z_i}\right)^2}{\sum_{i=1}^M \left(\frac{1}{1-z_i}\right)^2}.$$
 (25)

In the limit $M \to \infty$, the parameters \bar{n}_M and k_M coincide of course with the standard parameters of the not-truncated distributions.

One question still to be answered concerns the multiplicity of zeroes of the algebraic equation (3), both in general and in the specific case of the NB (Pascal) MD. Let us consider two polynomials S(z) and T(z) of degree m and n respectively:

$$S(z) = s_0 z^m + s_1 z^{m-1} + \dots + s_m \quad (s_0 \neq 0)$$

and

$$T(z) = t_0 z^n + t_1 z^{n-1} + \dots + t_n \quad (t_0 \neq 0)$$

It is known that S(z) and T(z) possess a not constant common factor iff the determinant

is equal to zero.

It follows that, called S' the first derivative of the polynomial S(z) with respect to z, S(z) will have at least one double root iff $R_{S,S'}=0$. In order

to be sure that the zeroes of a M-truncated generating function $G_M(z)$ are all distinct, it is therefore sufficient to show that none of the M roots z_i is such that $G_M(z_i) = G'_M(z_i) = 0$.

By rewriting $P_n^{[NB]}(\bar{n}, k)$ for simplicity in terms of parameters a and b (see equation (19) for the definition of a), one has

$$P_n^{[NB]}(a,b) = \frac{1}{n!}a(a+b)\dots(a+b(n-1))P_0,$$
(26)

and by properly normalising $G_M(z)$ one finds, by induction,

$$R_{G_M^{[NB]}, G_M'^{[NB]}} = A_M^{[NB]} \frac{a^M [(a+b)(a+2b)\dots(a+Mb)]^{M-1} P_0^{M-1}}{(M!)^{M-1}}.$$
 (27)

Since clearly $R_{G_M^{[NB]},G_M^{[NB]}}$ is always positive for a and b greater than zero, it follows that all the zeroes of the algebraic equation $G_M^{[NB]}(z)=0$ are distinct. Since all zeroes of $G_M^{[NB]}(z)=0$ are distinct, M conditions are needed to uniquely determine the set of zeroes. For k=1 for instance, one should expect that

$$\sum_{i=1}^{M} u_i = \sum_{i=1}^{M} u_i^2 = \dots = \sum_{i=1}^{M} u_i^M = -1.$$

In fact, from (16)

$$\sum_{i=1}^{M} u_i = -\frac{c_{M-1}^{[NB]}}{c_M^{[NB]}} = -\frac{M}{M+k-1} \xrightarrow{k \to 1} -1.$$

The same limit is obtained for

$$\sum_{i=1}^{M} u_i^2 = \left(-\frac{c_{M-1}^{[NB]}}{c_M^{[NB]}}\right)^2 - 2\frac{c_{M-2}^{[NB]}}{c_M^{[NB]}} \xrightarrow{k \to 1} -1$$

as well as for the other powers up to M. Notice that the same conditions are satisfied for $M \to \infty$ and constant k: consequently, also in this case the zeroes stay on the circle of unit radius, as will be discussed in the following.

3 Maps of zeroes for different classes of events in the rescaled complex z-plane.

We propose in this Section to apply the previously discussed theorems and remarks to the study, in the rescaled complex z-plane (i.e., in the complex u-plane), of maps of zeroes of the algebraic equations obtained by truncating at

integer value M the NB (Pascal) MD generating function. This distribution is used in a statistical model of multiparticle production to describe different classes of events (or substructures) in different collisions. These substructures are for instance 2- and 3-jets events in e^+e^- annihilation or events without mini-jets (soft events) and with mini-jets (semi-hard events) in pp collisions. Recently [9], in pp collisions, the occurrence of a third class of hard events at 14 TeV c.m. energy has been postulated also in the framework of the weighted superposition mechanism of different classes of events, each described by a NB (Pascal) MD with characteristic NB parameters. The occurrence of this third class of events was motivated by the fact that, by assuming both strong KNO scaling violations and QCD behaviour, extrapolations of NB parameters in the LHC energy domain implied, in the semi-hard sample of events, a surprising reduction in the average number of clans [8].

In order to deepen the analysis of the properties of collective variables in terms of the maps of complex zeroes and in order to study the possible occurrence of a phase transition, we focus our attention on the three mentioned classes of events at 14 TeV c.m. energy in pp collisions. Accordingly, the NB parameters used in the following are those described in [9]: $k_{soft} = 7$, $\bar{n}_{soft} = 40$, $k_{semi-hard} = 3.7$, $\bar{n}_{semi-hard} = 87$, $k_{hard} = 0.1212$, $\bar{n}_{hard} = 460$.

We find that for the soft and semi-hard components, the parameter k is greater than one and the zeroes stay *inside* the circle of unit radius in the complex u-plane (see Figures 1a and 1b). For the hard component, the parameter k is smaller than one and all the zeroes lie *outside* the circle of unit radius |u| = 1 (see Figure 1c). In order to make our statements more transparent, in Figures 2a, 2b, 2c the behaviour of the three classes of events in the region around the point u = 1 has been magnified for different cutoffs but fixed value of k. In Figure 3 the above maps are shown together close to the point u = 1, with the same fixed cut-off for three values of k corresponding to the three classes of events.

Notice that for k=1 all the zeroes stay on the circle of unit radius with the u=1 point excluded. In addition, when $M\to\infty$ the distribution of the zeroes of the algebraic equation obtained from the truncated and rescaled generating function converges towards the u=1 point for all classes of events with both k>1 and k<1.

As mentioned in the Introduction, in order to test the occurrence of a phase transition one has to find the behaviour of the zeroes of the grand canonical partition function \mathcal{Q} in the thermodynamical limit, i.e., with the size of the system going to infinity. The discussion is based on the approach contained in [1], where the generating function G(z) has been related to \mathcal{Q} by

$$Q = [G(0)]^{-1}. (28)$$

Relation (28) implies that the zeroes of the M-truncated grand canonical partition function \mathcal{Q}_M can be obtained from the zeroes of the M-truncated generating function G_M simply by rescaling those zeroes by a factor b (which was identified in [1] —it should be stressed again— with the fugacity).

The behaviour of the zeroes will then depend on the volume and the number of particles: when the MD is of NB type, as we are using now, it is sufficient to know the behaviour of the NB parameters. At present however, a realistic link between k and \bar{n} and the system size (the volume) is under investigation, hence postponed to a forthcoming paper. Here we limit ourselves to explore what happens when the thermodynamical limit corresponds to M (and \bar{n}) going to infinity with k fixed. In the first place we will check whether the EK theorem can be used to confine the zeroes to a narrowing region of the complex plane. Recalling Eq. (18), we notice that for k=1 one has $r[n]=\frac{1}{b}$. Thus minimum and maximum radii coincide and all the zeroes of $G_M(z)$ lie on a circle of radius 1/b, independently of the chosen cut-off M. Numerical studies show that the opening around the positive real axis is reduced when $M \to \infty$; this suggests that z = 1/b is an accumulation point of zeroes. It means of course that in this scenario for k=1, the point u=1 is an accumulation point of zeroes of the grand canonical partition function: since u on the real axis coincides with the fugacity, only for $b \to 1$ will a phase transition take place. For k > 1 the zeroes of the grand canonical partition function obey the following relation

$$r[n_{\min}] = \frac{1}{k} \le |u| \le r[n_{\max}] = \frac{M+1}{M+k}$$
 (29)

while for k < 1 the two limits are exchanged. Such a region does not shrink. We have to rely again on numerical root-finding, which still indicates the closing in of the zeroes to u = 1 (see Figures 1 and Figures 2), and at the same time shows that they are much closer together than the bound given by relation (29) allows. This feature again points in the direction of the presence of a possible phase transition at $b \to 1$.

In conclusion, the use of the rescaled complex variable u = bz marks visibly the different behaviour of the map of zeroes of the hard class of events with respect to the maps of the soft and semi-hard ones in our statistical model. In addition, it leads to identify the coefficients $c_n^{[NB]}$ of Eq. (16) with the canonical partition function for a system of n particles, and $H_M(u)$ with the truncated grand canonical partition function of the same system (in this framework $c_1 = k$, i.e., the parameter k coincides with the canonical partition function for a system with one particle, see also [1]). It should also be pointed out that in the rescaled version of this approach the NB parameter k alone controls the geometry of the distribution of the zeroes. This is indeed a quite

general property which is expected to be valid also in other collisions and especially in those collisions involving events with large numbers of particles, like heavy ion collisions. Finally, it has been shown that the NB parameter k is equal to minus the sum of the inverse of the zeroes, independently of the value of the cut-off M.

All these facts suggest to investigate further the thermodynamical content of the NB parameter k, and especially its dependence on temperature and volume, in view of a possible phase transition in the $b \to 1$ limit. Being indeed the fugacity $b = e^{\mu/k_BT}$ (with μ the chemical potential), one finds that μ goes to 0 in the limit $b \to 1$: this is a situation which is reached in a high temperature and high density real boson gas and which is expected to occur in a quark-gluon plasma.

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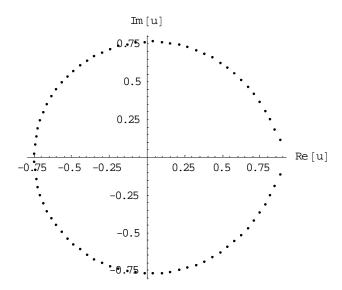


Fig. 1a: rescaled map of zeroes, in the complex u-plane, of the NB (Pascal) MD at 14 TeV c.m. energy with $k_{soft} = 7$ and cut-off M = 80 (M has been taken equal to $2\bar{n}_{soft}$). Zeroes lie inside the circle of unit radius |u| = 1.

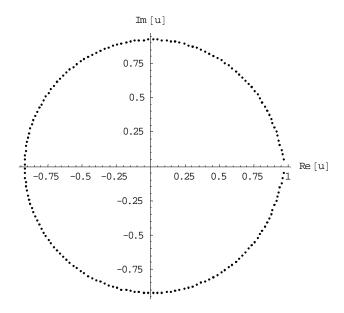


Fig. 1b: rescaled map of zeroes, in the complex u-plane, of the NB (Pascal) MD at 14 TeV c.m. energy with $k_{semi=hard}=3.7$ and cut-off M=174 (M has been taken equal to $2\bar{n}_{semi=hard}$). Zeroes lie inside the circle of unit radius |u|=1.

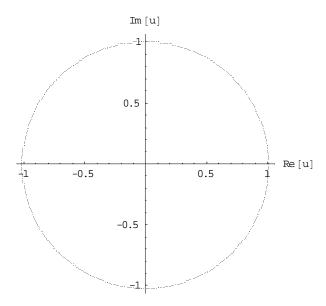


Fig. 1c: rescaled map of zeroes, in the complex u-plane, of NB (Pascal) MD at 14 TeV c.m. energy with $k_{hard}=0.1212$ and cut-off M=600. Zeroes lie outside the circle of unit radius |u|=1.

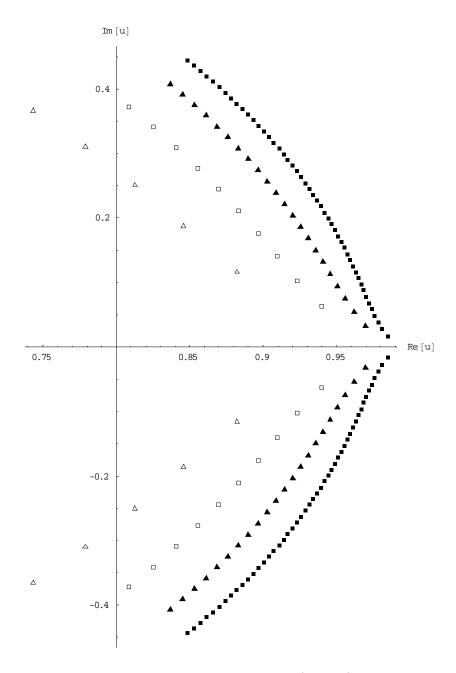


Fig. 2a: the rescaled map of zeroes of the NB (Pascal) MD of Fig. 1a has been magnified around the point u=1 for different cut-offs M (white and black triangles correspond to M=80 and M=320 respectively, and white and black squares to M=160 and M=640). As M increases, the point u=1 is shown to become an accumulation point of zeroes from the inside.

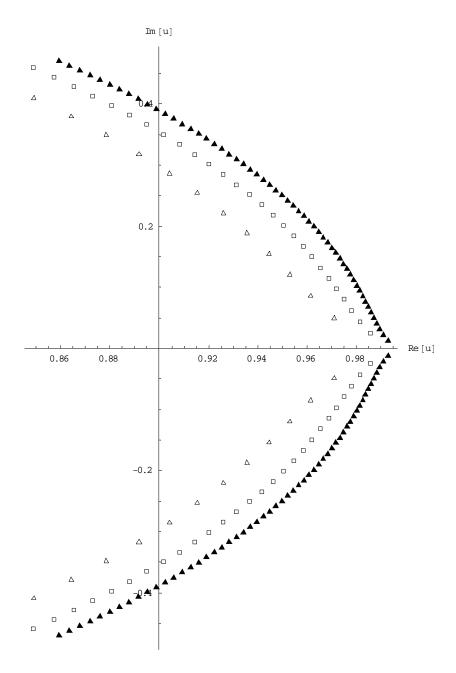


Fig. 2b: the rescaled map of zeroes of the NB (Pascal) MD of Fig. 1b has been magnified around the point u=1 for different cut-offs M (white triangles correspond to M=174, white squares to M=348 and black triangles to M=696). As M increases, the point u=1 is shown to become an accumulation point of zeroes from the inside.

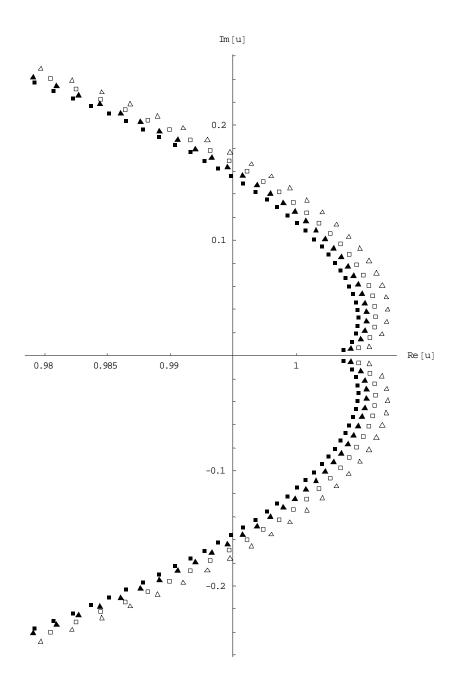


Fig. 2c: the rescaled map of zeroes of the NB (Pascal) MD of Fig. 1c has been magnified around the point u=1 for different cut-offs M (white triangles and squares correspond to M=600 and M=700 respectively, and black triangles and squares to M=800 and M=920). As M increases, the point u=1 is shown to become an accumulation point of zeroes from the outside.

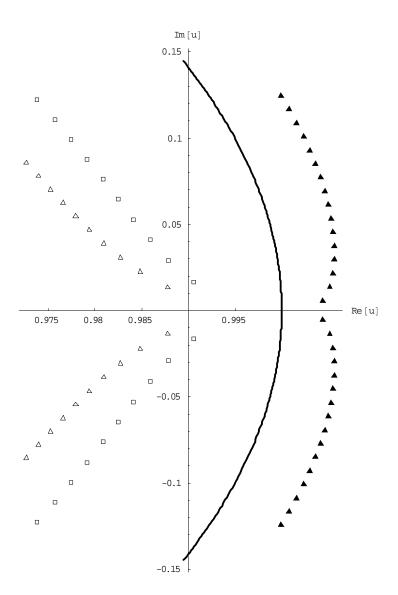


Fig. 3: maps of zeroes of the NB (Pascal) MD are shown for different values of the parameter k and the same fixed cut-off M=800. White triangles correspond to k_{soft} of Fig. 1a, white squares to $k_{semi-hard}$ of Fig. 1b and black triangles to k_{hard} of Fig. 1c. The full line describes the circle of unit radius |u|=1. The figure illustrates that —as discussed in the text—the point u=1 is an accumulation point of zeroes from the inside (for k>1) and from the outside (for k<1.)